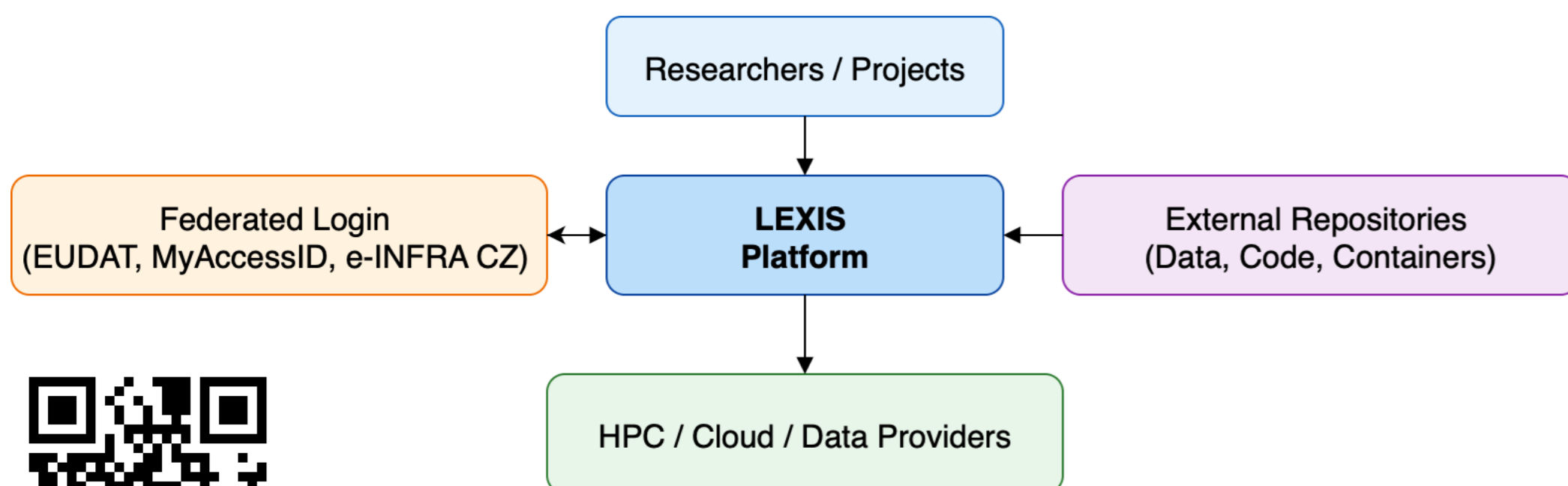


LEXIS Platform

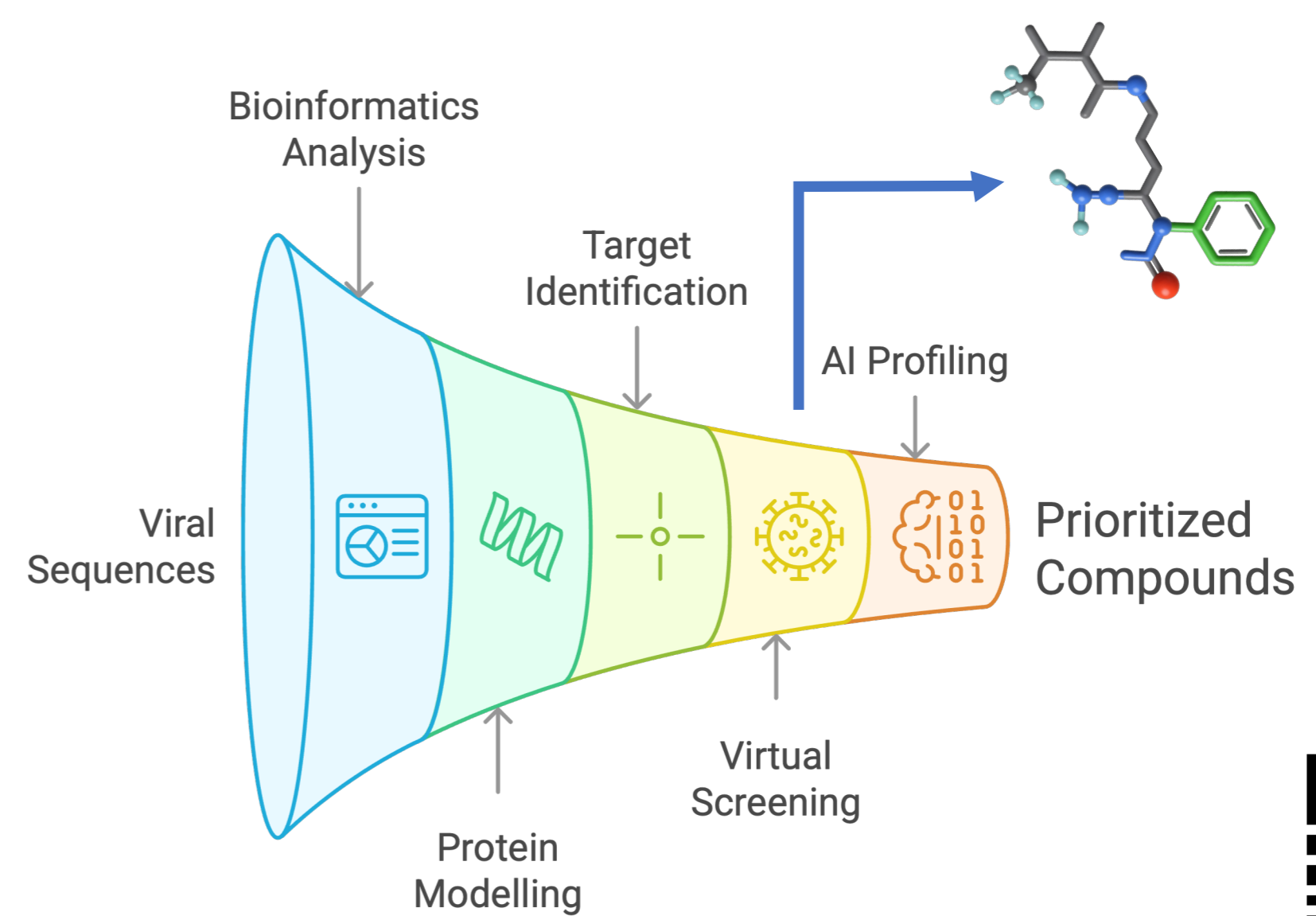
- Provides a **unified portal** for HPC workflows and data management.
- Supports **Federated login** (EUDAT, MyAccessID, e-INFRA CZ).
- Federates European computing centres**, bridging HPC, cloud, and data providers.
- Simplifies **project management**: users, datasets, workflows, and resources.
- Enables **workflow orchestration** with seamless job submission and monitoring (GUI or API).
- Ensures **secure access** via Federated Authentication & Authorization Infrastructure (AAI).



LEXIS Platform

Scalable Virtual Screening

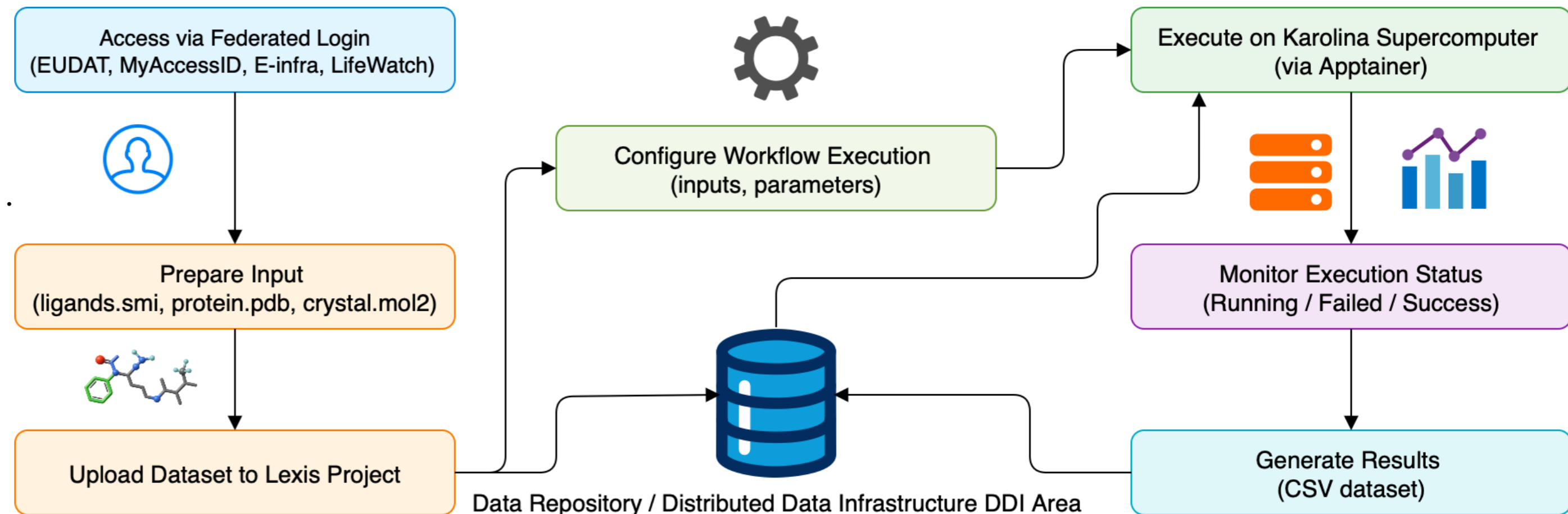
- High-performance **docking** software developed by Dompé.
- Designed for **HPC** environments; scales to millions of ligands.
- Accelerates drug discovery through fast **ligand-protein screening**.
- Part of the EXSCALATE platform for **urgent computing scenarios**.
- Generates ligand **scores** enabling downstream ranking and validation.



HPC-VS Interface

HPC-Accelerated Virtual Screening with the LEXIS Platform

- User authentication via **Federated login**.
- Input data uploaded in a **standardized format**.
- Workflow execution configured through **GUI or CLI**.
- Jobs executed on **Karolina** via **Apptainer**.
- Real time monitoring** through LEXIS.
- Results retrieved as **structured datasets** (CSV).



Ergonomic User Interface with Flexible and Intuitive Actions

- Flexible and ergonomic user interface that **simplifies access to virtual screening**.
- User oriented** data upload, job execution, and **seamless access to outputs**.



Demo Video

Upload data via web portal

Launch and monitor execution

Retrieve and download results

